

ring nodes : chain bonds :

33-38 ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 28-29 28-33 29-30 30-31 31-32 32-33 exact/norm bonds :

1-18 2-25 3-26 4-7 5-17 6-24 9-10 11-12 11-13 18-28 20-21 29-36 30-35 31-34 32-37 33-38

normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 28-29 28-33 29-30 30-31 31-32 32-33

G1:[@1],[@2]

G2:H,X,Ak,[@1],[@2],[@3]

G3:C,O,S

Hydrogen count : 7:>= minimum 1 34:>= minimum 1

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS